LA-UR-05-8430

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Title: Comparison of ENDF/B-VI and Initial ENDF/B-VII Results for the MCNP Criticality Validation Suite

Author(s): Russell D. Mosteller

Submitted to: 2005 Winter Meeting of the American Nuclear Society
November 12 - 17, 2005
Washington, DC

Los Alamos NATIONAL LABORATORY

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Comparison of ENDF/B-VI and Initial ENDF/B-VII Results for the MCNP Criticality Validation Suite

Russell D. Mosteller

Diagnostics Applications Group (X-5)
Applied Physics Division
Los Alamos National Laboratory

To Be Presented at the 2005 Winter Meeting of the American Nuclear Society
Washington, DC November 13 - 17, 2005

An assessment of the reactivity impact of some nuclear data proposed for the initial release of ENDF/B-VII has been made using the MCNP criticality validation suite. Relative to ENDF/B-VI, the changes primarily involve high-energy data for the uranium isotopes and ^{239}Pu, resonance parameters for ^{233}U, ^{235}U, and ^{238}U, and the 1/v thermal tail for hydrogen.

Four sets of calculations were performed for the MCNP Criticality Validation Suite using the MCNP5 Monte Carlo code. The first set employed nuclear data from ENDF/B-VI Release 8, the final release for ENDF/B-VI. The second set employed the T16_2003 nuclear data library that was distributed as part of an interim release of MCNP5 in the summer of 2004. The third set used nuclear data generated by group T-16 at Los Alamos National Laboratory for the initial release of ENDF/B-VII, and the fourth set employed the JENDL-3.3 library for MCNP that has recently become available. This presentation omits the T16_2003 results, but they are included in the abstract published in the Transactions for this meeting.

The results from the calculations demonstrate that the ENDF/B-VII changes produce substantial overall improvements relative to ENDF/B-VI and JENDL-3.3. In particular, the calculated ENDF/B-VII results differ from the corresponding benchmark values by more than two standard deviations for only five of the 31 cases in the suite, compared to nine cases for both the ENDF/B-VI and JENDL-3.3 data. Furthermore, the ENDF/B-VI and JENDL-3.3 data each produce statistically better results than the ENDF/B-VII data for only three cases, whereas the ENDF/B-VII data produce statistically better results than ENDF/B-VI and JENDL-3.3 for ten and twelve cases, respectively .

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Applied Physics Division
Los Alamos National Laboratory
mosteller@ lanl.gov

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OVERVIEW OF PRESENTATION

Succinct Description of MCNP Criticality Validation Suite

Characteristics of Preliminary Nuclear Data for ENDF/B-VII

Comparison of Results from MCNP5 Using JENDL-3.3, ENDF/B-VI and Initial ENDF/B-VII Nuclear Data Libraries

Conclusions

MCNP Criticality Validation Suite

Cases were selected to encompass a wide variety of

Fissile isotopes	:	^{233}U, ^{235}U, and ^{239}Pu
Spectra	:	Fast, intermediate, and thermal
Compositions	:	Metals, oxides, and solutions
Configurations	:	Bare and reflected spheres and cylinders, 2-D and 3-D lattices, and infinite homogeneous and heterogeneous regions

^{235}U Cases were subdivided into HEU, IEU, AND LEU

Input specifications for all 31 cases are taken from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments*

CASES IN THE MCNP CRITICALITY VALIDATION SUITE

Spectrum	Fast			Intermed	Thermal	
Geometry	Bare	Heavy Reflector	Light Reflector	Any	Lattice of Fuel Pins	Solution
^{233}U	Jezebel-233	Flattop-23	U233-MF-05	Falstaff-1*	SB-2½	ORNL-11
HEU	Godiva Tinkertoy-2	Flattop-25	Godiver	Zeus-2 UH_3	SB-5	ORNL-10
IEU	IEU-MF-03	BIG TEN	IEU-MF-04	Zebra-8H†	IEU-CT-02	STACY-36
LEU					B&W XI-2	LEU-ST-02
Pu	Jezebel Jezebel-240 Pu Buttons	Flattop-Pu THOR	Pu-MF-11	HISS/HPG†	PNL-33	PNL-2

* Extrapolated to critical † k_∞ measurement

CASES IN THE CRITICALITY VALIDATION SUITE

Name	Spectrum	*Handbook* ID	Description
Jezebel-233	Fast	U233-MET-FAST-001	Bare sphere of ^{233}U
Flattop-23	Fast	U233-MET-FAST-006	Sphere of ^{233}U reflected by normal U
U233-MF-05	Fast	U233-MET-FAST-005, case 2	Sphere of ^{233}U reflected by beryllium
Falstaff-1	Intermediate	U233-SOL-INTER-001, case 1	Sphere of uranyl fluoride solution enriched in ^{233}U
SB-2½	Thermal	U233-COMP-THERM-001, case 3	Lattice of ^{233}U fuel pins in water
ORNL-11	Thermal	U233-SOL-THERM-008	Large sphere of uranyl nitrate solution enriched in ^{233}U
Godiva	Fast	HEU-MET-FAST-001	Bare HEU sphere
Tinkertoy-2	Fast	HEU-MET-FAST-026, case C-11	3 x 3 x 3 array of HEU cylinders in paraffin box
Flattop-25	Fast	HEU-MET-FAST-028	HEU sphere reflected by normal U
Godiver	Fast	HEU-MET-FAST-004	HEU sphere reflected by water
Zeus-2	Intermediate	HEU-MET-INTER-006, case 2	HEU platters moderated by graphite and reflected by copper
UH_3	Intermediate	HEU-COMP-INTER-003, case 6	UH_3 cylinders reflected by depleted uranium
SB-5	Thermal	U233-COMP-THERM-001, case 6	Lattice of HEU fuel pins in water, with blanket of ThO_2 pins
ORNL-10	Thermal	HEU-SOL-THERM-032	Large sphere of HEU nitrate solution
IEU-MF-03	Fast	IEU-MET-FAST-003	Bare sphere of IEU (36 wt.%)
BIG TEN	Fast	IEU-MET-FAST-007	Cylinder of IEU (10 wt.%) reflected by normal uranium
IEU-MF-04	Fast	IEU-MET-FAST-004	Sphere of IEU (36 wt.%) reflected by graphite
Zebra-8H	Intermediate	MIX-MET-FAST-008, case 7	IEU (37.5 wt.%) reflected by normal U and steel
IEU-CT-02	Thermal	IEU-COMP-THERM-002, case 3	Lattice of IEU (17 wt.%) fuel rods in water
STACY-36	Thermal	LEU-SOL-THERM-007, case 36	Cylinder of IEU (9.97 wt.%) uranyl nitrate solution
B&W XI-2	Thermal	LEU-COMP-THERM-008, case 2	Large lattice of LEU (2.46 wt.%) fuel pins in borated water
LEU-ST-02	Thermal	LEU-SOL-THERM-002, case 2	Sphere of LEU (4.9 wt.%) uranyl fluoride solution
Jezebel	Fast	PU-MET-FAST-001	Bare sphere of plutonium
Jezebel-240	Fast	PU-MET-FAST-002	Bare sphere of plutonium (20.1 at.% ^{240}Pu)
Pu Buttons	Fast	PU-MET-FAST-003, case 103	3 x 3 x 3 array of small cylinders of plutonium
Flattop-Pu	Fast	PU-MET-FAST-006	Plutonium sphere reflected by normal U
THOR	Fast	PU-MET-FAST-008	Plutonium sphere reflected by thorium
PU-MF-11	Fast	PU-MET-FAST-011	Plutonium sphere reflected by water
HISS/HPG	Intermediate	PU-COMP-INTER-001	Infinite, homogeneous mixture of plutonium, hydrogen, and graphite
PNL-33	Thermal	MIX-COMP-THERM-002, case 4	Lattice of mixed-oxide fuel pins in borated water
PNL-2	Thermal	PU-SOL-THERM-021, case 3	Sphere of plutonium nitrate solution

PURPOSE AND USE OF THE MCNP CRITICALITY VALIDATION SUITE

The MCNP Criticality Validation Suite was developed to assess the reactivity impact of future improvements to MCNP as well as changes to its associated nuclear data libraries

Suite is *not* an absolute indicator of the accuracy or reliability of a given nuclear data library, nor is it intended to be

Suite can provide a general indication of the overall performance of a nuclear data library

Suite can provide an early warning of unexpected or unintended consequences resulting from changes to nuclear data

INITIAL NUCLEAR DATA FOR ENDF/B-VII

Final version of ENDF/B-VI (Release 8) was released in October 2001

JENDL-3.3 library for MCNP recently became available through RSICC

Are future nuclear data libraries likely to produce improved results?

Initial ENDF/B-VII changes (as of March 2005) to ^{1}H, ^{233}U, ^{235}U, ^{238}U, and ^{239}Pu offer encouragement

Data changes primarily involve:

- high-energy cross sections and data for the uranium isotopes and ^{239}Pu (LANL group T-16)
- revised resonance parameters for ^{233}U, ^{235}U, and ^{238}U (ORNL)
- slight reduction in 1/v thermal tail for ^{1}H capture cross section

MCNP5 CALCULATIONS FOR CRITICALITY VALIDATION SUITE

Each calculation employed 550 generations with 10,000 neutrons per generation (350 generations for SB-5 and Zebra-8H)

Results from first 50 generations were excluded from the statistics

Results therefore are based on 5,000,000 active histories for each case (3,000,000 for SB-5 and Zebra-8H)

ENDF/B-VI cross sections were used in ENDF/B-VII calculations for nuclides not included in the initial ENDF/B-VII set (i.e., everything except ^{1}H, ^{239}Pu, and the uranium isotopes)

ENDF/B-VI thermal scattering kernels (from SAB2002 library) were used for all three sets of calculations

RESULTS FOR ^{233}U BENCHMARKS

Case	Benchmark k_{eff}	Calculated k_{eff}		
		ENDF/B-VII	ENDF/B-VI	JENDL-3.3
Jezebel-233	1.0000 ± 0.0010	0.9997 ± 0.0003	0.9926 ± 0.0003	1.0041 ± 0.0003
Flattop-23	1.0000 ± 0.0014	0.9994 ± 0.0003	1.0003 ± 0.0003	0.9985 ± 0.0003
U233-MF-05	1.0000 ± 0.0030	0.9979 ± 0.0003	0.9972 ± 0.0003	1.0019 ± 0.0003
Falstaff-1	1.0000 ± 0.0083	0.9906 ± 0.0005	0.9895 ± 0.0005	0.9879 ± 0.0005
SB-2½	1.0000 ± 0.0024	0.9988 ± 0.0005	0.9964 ± 0.0005	0.9977 ± 0.0005
ORNL-11	1.0006 ± 0.0029	1.0041 ± 0.0002	0.9974 ± 0.0002	0.9989 ± 0.0002

$|\Delta k| \le \sigma$ $\qquad$ $\sigma < |\Delta k| \le 2\sigma$

k_{eff} for Jezebel-233 improves dramatically, and reactivity swing from Jezebel-233 to Flattop-23 is eliminated

k_{eff} for SB-2½ improves substantially relative to ENDF/B-VI

JENDL-3.3 produces best result for ORNL-11

RESULTS FOR HEU BENCHMARKS

Case	Benchmark k_{eff}	Calculated k_{eff}		
		ENDF/B-VII	ENDF/B-VI	JENDL-3.3
Godiva	1.0000 ± 0.0010	0.9994 ± 0.0003	0.9963 ± 0.0003	1.0033 ± 0.0003
Tinkertoy-2	1.0000 ± 0.0038	1.0004 ± 0.0003	0.9973 ± 0.0003	1.0042 ± 0.0003
Flattop-25	1.0000 ± 0.0030	1.0029 ± 0.0003	1.0021 ± 0.0003	0.9978 ± 0.0003
Godiver	0.9985 ± 0.0011	0.9978 ± 0.0004	0.9948 ± 0.0003	1.0018 ± 0.0004
UH_3	1.0000 ± 0.0047	0.9952 ± 0.0004	0.9914 ± 0.0003	0.9967 ± 0.0004
Zeus-2	0.9997 ± 0.0008	0.9958 ± 0.0004	0.9942 ± 0.0003	0.9967 ± 0.0003
SB-5	1.0015 ± 0.0028	0.9957 ± 0.0005	0.9965 ± 0.0005	0.9995 ± 0.0005
ORNL-10	1.0015 ± 0.0026	0.9989 ± 0.0002	0.9992 ± 0.0002	0.9999 ± 0.0002

k_{eff} improves substantially for Godiva, Godiver, and UH_3 but deteriorates slightly for SB-5

Reactivity swing from Godiva to Flattop-25 is reduced significantly

RESULTS FOR IEU BENCHMARKS

Case	Benchmark k_{eff}	Calculated k_{eff}		
		ENDF/B-VII	ENDF/B-VI	JENDL-3.3
IEU-MF-03	1.0000 ± 0.0017	1.0027 ± 0.0003	0.9987 ± 0.0003	0.9969 ± 0.0002
BIG TEN	0.9948 ± 0.0013	0.9952 ± 0.0002	1.0071 ± 0.0003	0.9851 ± 0.0002
IEU-MF-04	1.0000 ± 0.0030	1.0072 ± 0.0003	1.0036 ± 0.0003	1.0024 ± 0.0003
Zebra-8H	1.0300 ± 0.0025	1.0198 ± 0.0002	1.0406 ± 0.0002	1.0151 ± 0.0002
IEU-CT-02	1.0017 ± 0.0044	1.0008 ± 0.0003	1.0004 ± 0.0003	1.0018 ± 0.0003
STACY-36	0.9988 ± 0.0013	0.9994 ± 0.0003	0.9986 ± 0.0003	0.9999 ± 0.0003

k_{eff} improves dramatically for BIG TEN

k_{eff} is worse for IEU-MF-03 and IEU-MF-04 and drops substantially for Zebra-8H

For IEU-CT-02 and STACY-36, changes to resonance parameters offset reactivity effects of other changes for uranium isotopes

RESULTS FOR LEU BENCHMARKS

Case	Benchmark k_{eff}	Calculated k_{eff}		
		ENDF/B-VII	ENDF/B-VI	JENDL-3.3
B&W XI-2	1.0007 ± 0.0012	1.0000 ± 0.0003	0.9968 ± 0.0003	0.9991 ± 0.0003
LEU-ST-02	1.0024 ± 0.0037	0.9961 ± 0.0003	0.9953 ± 0.0003	0.9962 ± 0.0003

k_{eff} improves substantially for B&W XI-2, which eliminates need for *ad hoc* adjustment to ^{238}U resonance integral (used in many nuclear data libraries since early 1970s)

For LEU-ST-02, changes to resonance parameters offset reactivity effects of other changes for uranium isotopes

RESULTS FOR PU BENCHMARKS

Case	Benchmark k_{eff}	Calculated k_{eff}		
		ENDF/B-VII	ENDF/B-VI	JENDL-3.3
Jezebel	1.0000 ± 0.0020	0.9998 ± 0.0003	0.9971 ± 0.0003	0.9966 ± 0.0004
Jezebel-240	1.0000 ± 0.0020	1.0003 ± 0.0003	0.9980 ± 0.0003	1.0009 ± 0.0004
Pu Buttons	1.0000 ± 0.0030	0.9984 ± 0.0003	0.9962 ± 0.0003	0.9958 ± 0.0004
Flattop-Pu	1.0000 ± 0.0030	1.0004 ± 0.0003	1.0016 ± 0.0003	0.9904 ± 0.0003
THOR	1.0000 ± 0.0006	1.0079 ± 0.0003	1.0057 ± 0.0003	1.0066 ± 0.0003
Pu-MF-11	1.0000 ± 0.0010	0.9992 ± 0.0004	0.9966 ± 0.0004	0.9982 ± 0.0003
HISS/HPG	1.0000 ± 0.0110	1.0106 ± 0.0003	1.0106 ± 0.0003	1.0135 ± 0.0002
PNL-33	1.0024 ± 0.0021	1.0063 ± 0.0003	1.0029 ± 0.0003	1.0069 ± 0.0003
PNL-2	1.0000 ± 0.0065	1.0029 ± 0.0005	1.0033 ± 0.0005	1.0062 ± 0.0005

Striking improvement in k_{eff} for fast cases except THOR

Reactivity swing from Jezebel to Flattop-Pu is eliminated

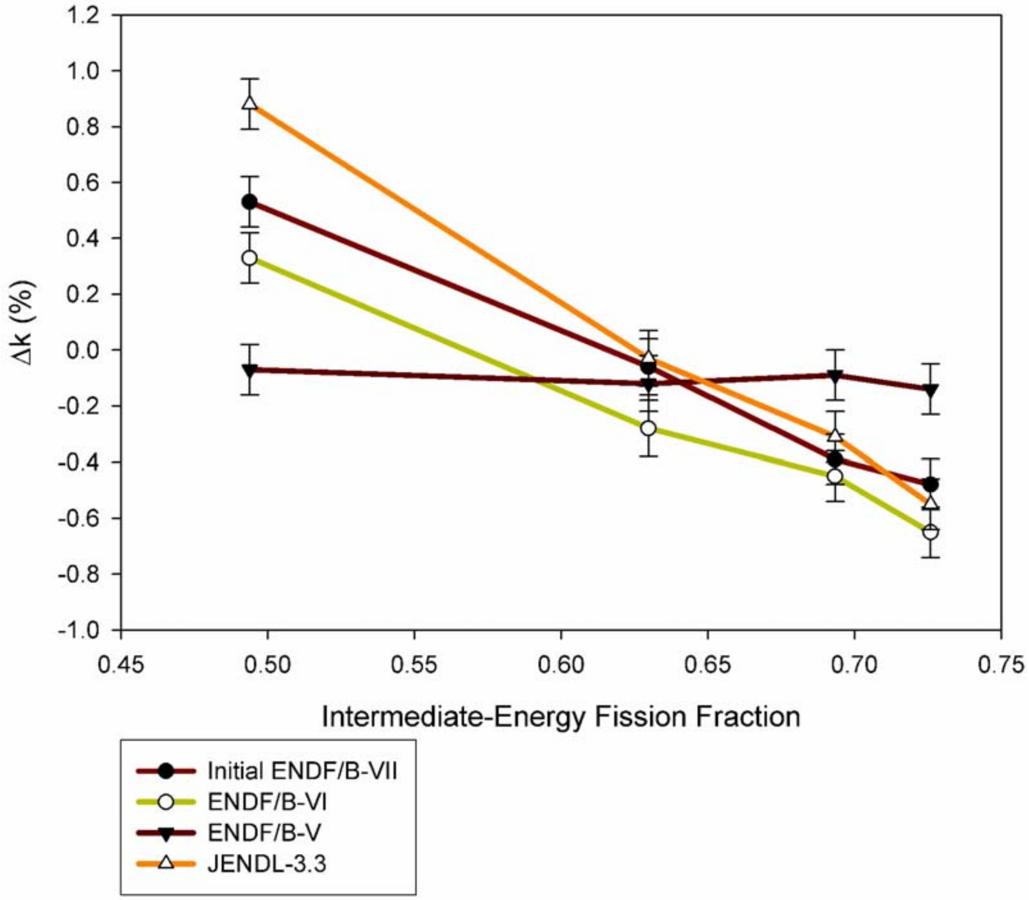
SUMMARY OF RESULTS FOR MCNP CRITICALITY VALIDATION SUITE

Range	ENDF/B-VII	ENDF/B-VI	JENDL-3.3
$\lvert\Delta k\rvert \leq \sigma$	21	13	13
$\sigma < \lvert\Delta k\rvert \leq 2\sigma$	5	9	9
$\lvert\Delta k\rvert > 2\sigma$	5	9	9

Substantial improvements for bare metal spheres (Jezebel-233, Godiva, and Jezebel), BIG TEN, HEU and Pu metal spheres in water (Godiver and Pu-MF-011, respectively), and LEU lattice (B&W XI-2)

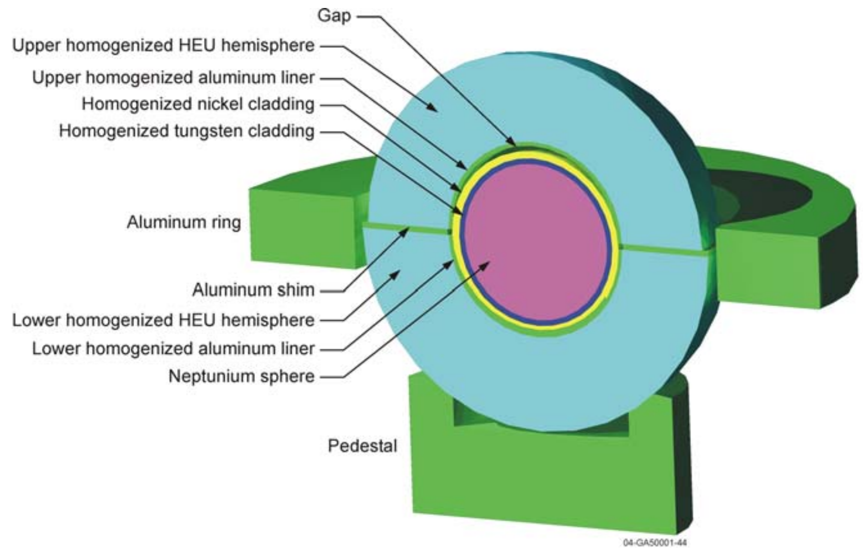
ORNL resonance parameters improve results for Godiver, ORNL-10, IEU-CT-03, STACY-36, B&W XI-2, and LEU-ST-02

ZEUS HEU-GRAPHITE BENCHMARKS



⇒ Cross sections for ^{235}U in the unresolved resonance region should be re-examined

NEPTUNIUM SPHERE REFLECTED BY HEU



Benchmark k_{eff}	Calculated k_{eff}		
	ENDF/B-VII	ENDF/B-VI	JENDL-3.3
1.0019 ± 0.0036	0.9924 ± 0.0003	0.9889 ± 0.0002	0.9967 ± 0.0002

$\sigma < |\Delta k| \leq 2\sigma$ $\qquad$ $|\Delta k| > 2\sigma$

⇒ Fast cross sections for ^{237}Np should be reviewed

UNMODERATED ZEUS BENCHMARK

Benchmark k_{eff}	Basic Library	Calculated k_{eff}	
		ENDF/B-VI Cu	ENDF/B-V Cu
1.0012 ± 0.0015	ENDF/B-VII	1.0108 ± 0.0003	1.0001 ± 0.0003
	ENDF/B-VI	1.0080 ± 0.0003	0.9968 ± 0.0003
	ENDF/B-V	1.0088 ± 0.0003	0.9960 ± 0.0003
	JENDL-3.3	1.0242 ± 0.0003*	1.0000 ± 0.0003

* JENDL-3.3 Cu

$|\Delta k| > 2\sigma$

Benchmark contains no moderator and therefore has a fast spectrum

Differences between ENDF/B-V and ENDF/B-VI Cu cross sections have little net reactivity impact on previous Zeus benchmarks, which have intermediate spectra

⇒ Fast cross sections for Cu should be reviewed

48-INCH SPHERE OF PLUTONIUM NITRATE SOLUTION

Benchmark k_{eff}	Calculated k_{eff}		
	ENDF/B-VII	ENDF/B-VI	JENDL-3.3
1.0003 ± 0.0033	1.0191 ± 0.0002	1.0189 ± 0.0002	1.0227 ± 0.0002

$|\Delta k| > 2\sigma$

Same sphere as for ORNL-10 (HEU) and ORNL-11 (^{233}U) Benchmarks

Very thermal spectra with very little leakage

⇒ Cross sections for ^{239}Pu (and probably ^{233}U) should be re-examined in the deep thermal range

RESULTS FOR HEAVY-WATER SOLUTIONS

Case	Benchmark k_{eff}	Calculated k_{eff}		
		ENDF/B-VII + JENDL-3.3 ^2H	Initial ENDF/B-VII	JENDL-3.3
Reflected Spheres (HEU-SOL-THERM-004)				
1	1.0000 ± 0.0033	0.9947 ± 0.0004	0.9839 ± 0.0004	0.9918 ± 0.0004
2	1.0000 ± 0.0036	0.9911 ± 0.0004	0.9795 ± 0.0004	0.9873 ± 0.0004
3	1.0000 ± 0.0039	0.9975 ± 0.0004	0.9862 ± 0.0004	0.9979 ± 0.0004
4	1.0000 ± 0.0046	0.9998 ± 0.0004	0.9892 ± 0.0004	0.9971 ± 0.0004
5	1.0000 ± 0.0052	0.9972 ± 0.0004	0.9877 ± 0.0005	0.9956 ± 0.0004
6	1.0000 ± 0.0059	0.9936 ± 0.0004	0.9844 ± 0.0004	0.9913 ± 0.0004
Unreflected Cylinders (HEU-SOL-THERM-020)				
1	0.9966 ± 0.0116	1.0041 ± 0.0005	0.9915 ± 0.0005	1.0006 ± 0.0005
2	0.9956 ± 0.0093	1.0077 ± 0.0005	0.9973 ± 0.0005	1.0066 ± 0.0005
3	0.9957 ± 0.0079	1.0163 ± 0.0005	1.0059 ± 0.0005	1.0149 ± 0.0005
4	0.9955 ± 0.0078	1.0139 ± 0.0005	1.0023 ± 0.0005	1.0160 ± 0.0005
5	0.9959 ± 0.0077	1.0204 ± 0.0005	1.0091 ± 0.0005	1.0167 ± 0.0005

$\sigma < |\Delta k| \leq 2\sigma$ $|\Delta k| > 2\sigma$

CONCLUSIONS

Overall, initial ENDF/B-VII produces major reactivity improvements relative to ENDF/B-VI and JENDL-3.3

Reactivity swings from bare spheres to corresponding systems reflected by normal uranium are eliminated or substantially reduced

Need for *ad hoc* adjustment to ^{238}U resonance integral may be eliminated

Improvements still are needed, particularly for cases with

- intermediate spectra
- thorium
- neptunium
- copper and a fast spectrum
- plutonium and a thermal spectrum
- deuterium (possibly)